

1,2-Dichlorobenzene
95-50-1 | DTXSID6020430

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.90×10^{-11} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 2.72×10^{-1}

Confidence level: 6.62×10^{-1}

Nearest Neighbors from the Training Set

Image not found

(2E)-3-Phenylprop-2-enal

Measured: 4.80×10^{-11}

Predicted: 5.31×10^{-11}

Image not found

(E)-Crotonaldehyde

Measured: 3.61×10^{-11}

Predicted: 3.73×10^{-11}

Image not found

Crotonaldehyde

Measured: 3.61×10^{-11}

Predicted: 3.73×10^{-11}

Image not found

1,4-Naphthoquinone

Measured: 3.10×10^{-12}

Predicted: 3.16×10^{-11}

Image not found

1,3,5-Cycloheptatriene

Measured: 9.69×10^{-11}

Predicted: 1.00×10^{-10}

Image not found

(2E)-2-Hexenal

Measured: 4.40×10^{-11}

Predicted: 4.31×10^{-11}